

## Supplementary Information

for

### **Two co-crystalline $M(\text{hfac})_2(\text{IPhIN})_2 \bullet M(\text{hfac})_2$ ( $M = \text{Mn}, \text{Co}$ ) compounds with a bis(iminoylnitroxide) biradical: structure and magnetism**

Maria G. F. Vaz<sup>a\*</sup>, Handan Akpınar<sup>b</sup>, Guilherme P. Guedes<sup>a,c</sup>, Sauli Santos, Jr.<sup>d</sup>,  
Miguel A. Novak<sup>e</sup>, Paul M. Lahti<sup>b\*</sup>

<sup>a</sup>*Instituto de Química, Universidade Federal Fluminense, Niterói, RJ 24020-150, Brazil*

<sup>b</sup>*Department of Chemistry, University of Massachusetts, Amherst, Massachusetts 01003, USA*

<sup>c</sup>*Instituto de Ciências Exatas, Departamento de Química, Universidade Federal Rural do Rio de Janeiro, Seropédica, RJ, 23890-000 Brazil.*

<sup>d</sup>*Curso de Física, Universidade Federal de Goiás, Jataí, GO 75804-120, Brazil*

<sup>e</sup>*Instituto de Física, Universidade Federal do Rio de Janeiro, Rio de Janeiro, RJ 21941-972, Brazil*

**Table S1.** Selected angles (*deg*) for compounds **1** and **2**.

Atoms	(1) (M=Mn)	(2) (M=Co)
<i>Bond angles</i>		
O6A—M1A—O2A	81.78(12)	82 (3)
O6A—M1A—O3A	108.92(12)	92 (4)
O2A—M1A—O3A	95.40(12)	102 (4)
O6A—M1A—O1A	92.96(9)	106 (4)
O2A—M1A—O1A	105.32(9)	94 (3)
O3A—M1A—O1A	151.86(9)	158 (4)
O6A—M1A—O4A	170.18(12)	93 (4)
O2A—M1A—O4A	93.40(12)	173 (4)
O3A—M1A—O4A	79.95(12)	83 (4)
O1A—M1A—O4A	80.01(8)	84 (4)
O6A—M1A—O5A	91.76(9)	172 (4)
O2A—M1A—O5A	170.41(9)	93 (3)
O3A—M1A—O5A	79.94(9)	83 (4)
O1A—M1A—O5A	82.0	80 (3)
N1A—O2A—M1A	119.9(2)	121 (7)
N5A—O6A—M1A	119.7(2)	120(8)
<i>Torsion angles</i>		
N1A—C17A—C18A—C23A	43.0(2)	41(20)
N4A—C24A—C22A—C21A	-24.7(1)	-27(21)
N5A—C37A—C38A—C39A	48.8(5)	48(23)
N7A—C44A—C40A—C39A	-24.1(6)	-22(24)

**Figure S1.** Crystal packing of compound **1**. (a) Closest contacts  $N-O\cdots N_{\text{imino}}$  and (b) Short contacts  $I\cdots F$  and hydrogen bonding among nitroxide oxygen atom, imino nitrogen atom and coordinated water molecules to Mn1B ( $\text{vii}=1.5-x, 1/2-y, -z$ ). Fluorine, hydrogen and carbon atoms of  $\text{hfac}^-$  ligands were omitted for sake of clarity.

